

2-Methylheptane
592-27-8 | DTXSID2060460

Model Performance

Model

Data

Weighted KNN model					
5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 460

Global applicability domain: Inside

Local applicability domain index: 6.51e-01

Confidence level: 7.24e-01

Nearest Neighbors from the Training Set

Image not found

Dibenzofuran

Measured: 1510

Predicted: 14.2

Image not found

Dibenzothiophene

Measured: 1120

Predicted: 84.5

Image not found

1-Methoxynaphthalene

Measured: 162

Predicted: 11.2

Image not found

Methylcyclohexane

Measured: 186

Predicted: 233

Image not found

Dicyclopentadiene

Measured: 219

Predicted: 228